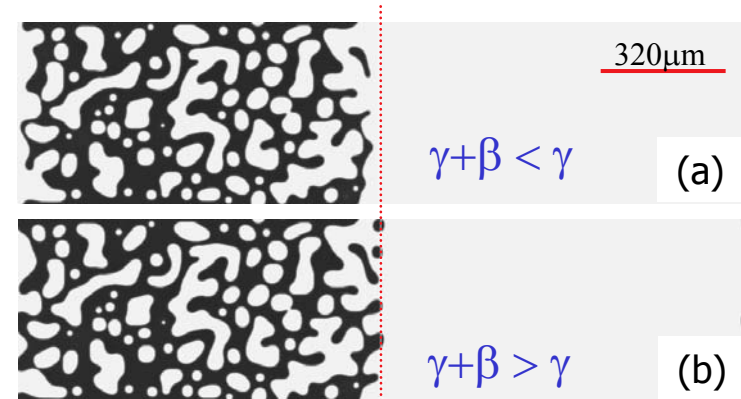


Computational Modeling of Interdiffusion Microstructures

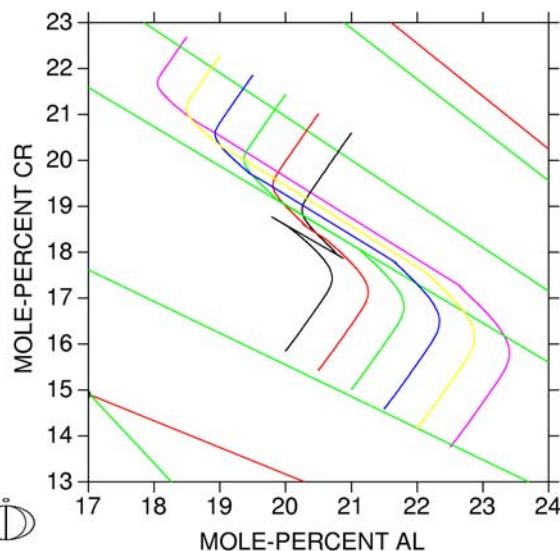
J. E. Morral, University of Connecticut, and Yunzhi Wang, Ohio State University
DMR - 0139705

Interdiffusion Predictions

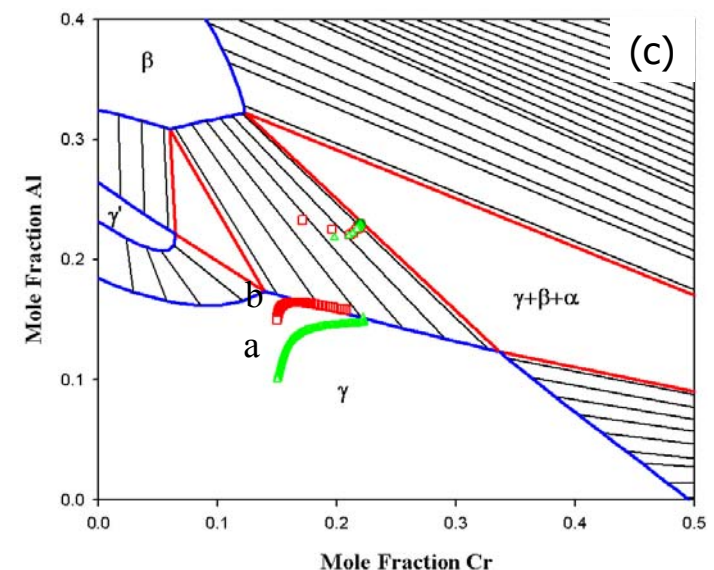
- A quantitative phase field model for interdiffusion in Ni-Al-Cr alloys was developed by using free energy and mobility databases created by the CALPHAD method. Microstructural changes (a) and (b) as well as diffusion paths (c) for two $\gamma+\beta/\gamma$ diffusion couples were predicted.



Annealing time: 25 hours



•DICTRA predictions of diffusion paths in $\gamma+\beta/\gamma+\beta$ diffusion couples showing the effect of initial alloy composition on the formation of "horns." (left figure). Horns can be seen in diffusion paths predicted by the phase field method, too (Figure (c)).



Computational Modeling of Interdiffusion Microstructures

J. E. Morral, University of Connecticut, and Yunzhi Wang, Ohio State University
DMR - 0139705

Presentations

- K. Wu, J. E. Morral and Y. Wang, "Microstructural Evolution in Interdiffusion Zones and Its Effects on Diffusion Path," TMS2005, 134th Annual Meeting and Exhibition, February 13-17, 2005, Moscone Convention Center, San Francisco, California (**Invited**).
- K. Wu, J. E. Morral and Y. Wang, "Quantitative Phase Field Modeling of Interdiffusion Microstructures in Multi-Phase and Multi-Component Alloys," TMS2004, 133rd Annual Meeting and Exhibition, March 14-18, 2004, Charlotte Convention Center, Charlotte, North Carolina (**invited**).
- Y. Wang, "Quantitative Phase Field Modeling of Microstructural Evolution," Max Planck Institute for Iron Research, Dusseldorf, Germany, August 25, 2003 (**invited**).
- J. E. Morral, Application of Local Equilibrium Principles to Modeling the Internal Oxidation and Failure of Fe-Cr-Al alloys, invited talk at the Gordon Research Conference on High Temperature Oxidation, New London, NH, July 20-25, 2003 (**invited**).

Publications

- K. Wu, J. E. Morral and Y. Wang, "Movement of Kirkendall Markers, Second Phase Particles and Type 0 Boundary in Two-Phase Diffusion Couple Simulations," *Acta mater.* **52**:1917-1925 (2004).
- K. Wu, Y. A. Chang and Y. Wang, "Simulating Interdiffusion Microstructure in Ni-Al-Cr Diffusion Couples: A Phase Field Approach Coupled with CALPHAD Database," *Scripta mater.* **50**:1145-1150 (2004).
- K. Wu, "Computer Simulation of Interdiffusion Microstructures in Multi-Component and Multiphase Systems," Ph.D. dissertation, The Ohio State University, 2003.